A "refined Born approximation" and Aitken's Δ^2 method

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ABSTRACT

Rayski has suggested methods for calculating scattering amplitudes, which are based on the use of parameterized wave functions in a Born expansion. It is shown that his one-parameter methods are equivalent to Aitken's Δ^2 transformation applied to successive elements of a Born sequence. Many-parameter variants are also discussed.

1. INTRODUCTION

In a recent paper Rayski [4] suggested the use of a parameterized wave function as the basis for a Born expansion in quantum mechanical scattering problems. The idea is to try to use the freedom of choice of parameter values to obtain an improved approximation for the scattering amplitude or phase shift when the ordinary Born sequence converges slowly. Iteration-variation methods are also based on the use of parameterized wave functions, the parameters in this case being determined by a variational principle, and these methods have been shown [2] to be equivalent to well-known sequence-to-sequence transformations. In this paper we show that Rayski's one-parameter methods are simply applications of Aitken's Δ^2 method to elements of a Born sequence of approximations.

2. THEORY

To facilitate comparison with Rayski's paper [4] some of his notation is adopted here. We are interested in a non-relativistic scattering problem described by the Schrödinger equation

$$(\nabla^2 + p^2)\, \psi(\underset{\sim}{r}) = U(r)\, \psi(\underset{\sim}{r}) . \tag{1}$$

The wave function, suitably normalized, may be expressed as

$$\psi(\underset{\sim}{r}) = \exp(i\, \underset{\sim}{p} \cdot \underset{\sim}{r}) + \gamma(\underset{\sim}{r}) ,$$

and γ then satisfies the integral equation

$$\gamma(\underset{\sim}{r}) = \int d\underset{\sim}{r}'\, G(\underset{\sim}{r}, \underset{\sim}{r}')\, U(r')\, [\exp(i\, \underset{\sim}{p} \cdot \underset{\sim}{r}') + \gamma(\underset{\sim}{r}')]$$

where $G(\underset{\sim}{r}, \underset{\sim}{r}')$ is the appropriate Green's function (see e.g. [3], p. 222). The Born sequence of approximations for γ is obtained by taking

$$\gamma_B^{(0)}(\underset{\sim}{r}) = 0$$

$$\gamma_B^{(n+1)}(\underset{\sim}{r}) = \int d\underset{\sim}{r}'\, G(\underset{\sim}{r}, \underset{\sim}{r}')\, U(r')\, [\exp(i\, \underset{\sim}{p} \cdot \underset{\sim}{r}') + \gamma_B^{(n)}(\underset{\sim}{r}')], \quad (n = 0, 1, \ldots). \tag{2}$$

The scattering amplitude $f_B^{(n)}(\theta)$, at scattering angle θ, in the n^{th} Born approximation is then deduced from the asymptotic form

$$\gamma_B^{(n)}(\underset{\sim}{r}) \underset{r \to \infty}{\sim} \frac{e^{ipr}}{r}\, f_B^{(n)}(\theta) .$$

In an attempt to obtain a more rapidly convergent sequence, Rayski [4] suggests the modified iterative process

$$\gamma^{(0)}(\underset{\sim}{r}) = a \exp(i\, \underset{\sim}{p} \cdot \underset{\sim}{r})$$

$$\gamma^{(n+1)}(\underset{\sim}{r}) = \int d\underset{\sim}{r}'\, G(\underset{\sim}{r}, \underset{\sim}{r}')\, U(r')[\exp(i\, \underset{\sim}{p} \cdot \underset{\sim}{r}') + \gamma_B^{(n)}(\underset{\sim}{r}')], \quad (n = 0, 1, \ldots) \tag{3}$$

which reduces to (2) when $a = 0$. Noting that

$$\gamma^{(1)}(\underset{\sim}{r}) = (1 + a)\, \gamma_B^{(1)}(\underset{\sim}{r})$$

and

$$\gamma^{(2)}(\underset{\sim}{r}) = (1 + a)\, \gamma_B^{(2)}(\underset{\sim}{r}) - a\, \gamma_B^{(1)}(\underset{\sim}{r}) ,$$

it is readily seen that

$$\gamma^{(n)}(\underset{\sim}{r}) = (1 + a)\, \gamma_B^{(n)}(\underset{\sim}{r}) - a\, \gamma_B^{(n-1)}(\underset{\sim}{r}) \tag{4}$$

for $n = 1, 2, \ldots$. The resulting scattering amplitude is

$$f^{(n)}(\theta) = (1 + a)\, f_B^{(n)}(\theta) - a\, f_B^{(n-1)}(\theta) . \tag{5}$$

Rayski uses two different ways of choosing a, which he calls asymptotic fitting and fitting at the origin :

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(a) Asymptotic fitting

Here α is chosen so that

$$f^{(n)}(\theta) = f^{(n-1)}(\theta)$$

for some n. It can be seen from (5) that this gives

$$\alpha = \frac{f_B^{(n-1)}(\theta) - f_B^{(n)}(\theta)}{f_B^{(n)}(\theta) - 2f_B^{(n-1)}(\theta) + f_B^{(n-2)}(\theta)} .$$

The scattering amplitude obtained in this way is

$$f^{(n)}(\theta) = \frac{f_B^{(n-2)}(\theta)\ f_B^{(n)}(\theta) - [f_B^{(n-1)}(\theta)]^2}{f_B^{(n)}(\theta) - 2f_B^{(n-1)}(\theta) + f_B^{(n-2)}(\theta)}$$

which is precisely the result of applying Aitken's Δ^2 transformation to the three successive iterates $f_B^{(n-2)}(\theta)$, $f_B^{(n-1)}(\theta)$ and $f_B^{(n)}(\theta)$ (see e.g. [2]).

(b) Fitting at the origin

In this case α is found by taking

$$\gamma^{(n)}(0) = \gamma^{(n-1)}(0)$$

which gives

$$\gamma^{(n)}(0) = \frac{\gamma_B^{(n-2)}(0)\ \gamma_B^{(n)}(0) - [\gamma_B^{(n-1)}(0)]^2}{\gamma_B^{(n)}(0) - 2\gamma_B^{(n-1)}(0) + \gamma_B^{(n-2)}(0)} .$$

Again $f^{(n)}(\theta)$ is given by (5) but α is such that the value of $\gamma^{(n)}$ at the origin is the result of applying Aitken's Δ^2 method to $\gamma_B^{(n-2)}(0)$, $\gamma_B^{(n-1)}(0)$ and $\gamma_B^{(n)}(0)$. Since it is the asymptotic form of $\gamma(\underset{\sim}{r})$, rather than its behaviour at the origin, that affects the scattering amplitude, it is hardly surprising that method (a) gives better results than method (b) in Rayski's example of zero-energy scattering by a square well potential.
A two-parameter method suggested in [4] consists of taking

$$\gamma^{(0)}(\underset{\sim}{r}) = (\alpha + \beta r) \exp (i\, \underset{\sim}{p} \cdot \underset{\sim}{r})$$

and requiring that

$$\gamma^{(2)}(0) = \gamma^{(1)}(0) = \gamma^{(0)}(0) .$$

Unlike the one-parameter methods, this does not represent an extrapolation of a Born sequence. The approach is open to criticism on the grounds that it introduces an unphysical asymptotic behaviour. Although it may give improved results for potentials of short range, as in Rayski's very simple example, this must be regarded as an *ad hoc* method rather than one of general applicability.
As an alternative two-parameter approach we could generalize (3) by taking

$$\gamma^{(0)}(\underset{\sim}{r}) = \alpha\, \gamma_B^{(1)}(\underset{\sim}{r}) + \beta\, \gamma_B^{(2)}(\underset{\sim}{r}) .$$

This gives

$$\gamma^{(n)}(\underset{\sim}{r}) = a\, \gamma_B^{(n+1)}(\underset{\sim}{r}) + b\, \gamma_B^{(n)}(\underset{\sim}{r}) + c\, \gamma_B^{(n-1)}(\underset{\sim}{r}) \qquad (n = 1, 2, \ldots)$$

with

$$a = \beta\ , \quad b = 1 + \alpha - \beta\ , \quad c = -\alpha\ ,$$

and

$$f^{(n)}(\theta) = a\, f_B^{(n+1)}(\theta) + b\, f_B^{(n)}(\theta) + c\, f_B^{(n-1)}(\theta). \qquad (6)$$

Using the conditions

$$f^{(n+1)}(\theta) = f^{(n)}(\theta) = f^{(n-1)}(\theta),$$

for some n, we find that a, b and c satisfy the linear equations

$$a + b + c = 1$$

$$a\Delta_{n+1} + b\Delta_n + c\Delta_{n-1} = 0$$

$$a\Delta_n + b\Delta_{n-1} + c\Delta_{n-2} = 0$$

where

$$\Delta_n = f_B^{(n+1)}(\theta) - f_B^{(n)}(\theta).$$

The coefficients a, b and c may then be expressed as quotients of determinants; inserting the results in (6) we obtain, after some rearrangement of the determinants,

$$f^{(n)}(\theta) = \frac{\begin{vmatrix} f_B^{(n-2)}(\theta) & f_B^{(n-1)}(\theta) & f_B^{(n)}(\theta) \\ \Delta_{n-2} & \Delta_{n-1} & \Delta_n \\ \Delta_{n-1} & \Delta_n & \Delta_{n+1} \end{vmatrix}}{\begin{vmatrix} 1 & 1 & 1 \\ \Delta_{n-2} & \Delta_{n-1} & \Delta_n \\ \Delta_{n-1} & \Delta_n & \Delta_{n+1} \end{vmatrix}} .$$

In the notation of [2] this is $e_2(f_B^{(n-2)})$, a particular case of the ϵ algorithm; as Wynn has shown [5] this may be computed by a simpler method than direct evaluation of the determinants. Many-parameter methods generated in a similar manner reproduce higher-order entries of the ϵ-table, which may also be identified as Padé approximants.

3. CONCLUSION

We have shown that Rayski's one-parameter methods are two different ways of applying Aitken's Δ^2 method

to a Born sequence, and that a natural many-parameter extension of Rayski's approach is equivalent to an application of the ϵ algorithm, which may be regarded as a generalization of Aitken's method. Only calculations of the scattering amplitude have been discussed, but the same conclusions apply when Rayski's method is used to estimate scattering phase shifts for individual partial waves.
Non-linear sequence-to-sequence transformations, of which Aitken's method is a particularly simple example, have been studied extensively in recent years; much of the relevant literature may be traced through Brezinski's recent book [1]. The findings of this paper, and of [2], suggest that progress in that area could be usefully exploited in quantum mechanical scattering calculations.

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